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Variational approach to Hamiltonian lattice theories

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A variational calculation of the vacuum energy of a Hamiltonian lattice theory is formulated in terms of a finite box Hamiltonian for a cluster of points. The box Hamiltonian contains surface terms which are proportional to order parameters of the system. It is tested on the Ising model and applied to $Z(N)$ spin models in $1+1$ and $2+1$ dimensions. $Z(3)$ is found to have an exceptional phase-transition structure. The application of the method to local gauge theories is discussed.

I. INTRODUCTION

We propose a variational method which is based on periodic test functions for the vacuum of a Hamiltonian lattice theory. The basic unit of this test function is a cluster of lattice points (or links) for which we define a box Hamiltonian. Rather than vary explicitly the wave function, we vary surface parameters which are introduced into the box Hamiltonian. These parameters are proportional to order parameters of the system and therefore have direct physical meaning. From the lattice point of view this method is similiar to the Bethe-Peierls approximation in statistical mechanics, but in spirit it is similiar to the Hartree approach to atomic physics problems. Since it is based on a product wave function this method cannot describe accurately the critical point where large-scale fluctuations are important. It provides, however, a systematic improvement over mean-field results and leads, in the ordered region, to a simple and accurate calculation of the vacuum energy density.

In Sec. II we describe and test the method on the Ising model in $1+1$ dimensions. We discuss the successes and shortcomings of this method, comparing the results with the known solution. In particular, we observe how the method improves with the increase in the size of the "box". Using the smallest box, i.e., a single lattice point, we employ a mean-field approximation to all $Z(N)$ spin models in Sec. III. $Z(3)$ shows a first-order phase transition. This is a problem in $1+1$ dimensions, and we show how the transition weakens with increasing size of the box. We comment on local gauge theories in Sec. III as well as in Sec. IV. The latter is devoted to a discussion of several aspects of the variational method. In the Appendix we supply, for the sake of completeness, some mathematical details which were stated without proof in the main text.

II. ISING MODEL IN 1+1 DIMENSIONS

We investigate a variational approach to a Hamiltonian lattice theory. In order to introduce and test the method we will start with its application to a soluble problem: the transverse-field Ising model in $D=1$ space dimension.[1] Let us define its Hamiltonian by

$$-H=\sum_i \sigma_1(i)+g\sum_i \sigma_3(i)\sigma_3(i+1), \tag{1}$$

where σ_1 and σ_3 are Pauli matrices associated with every point of a one-dimensional lattice of length $L\to\infty$. This is a self-dual model which has two phases and a critical point at $g=1$.[2] Its exact energy density (per site) is given by[1]

$$-E=\frac{1}{\pi}\int_0^\pi dk\,(1+g^2+2g\cos k)^{1/2}. \tag{2}$$

Our method is based on dividing the lattice into L/n boxes of size n and solving first the box Hamiltonian

$$-h_n=\sum_{j=1}^{n}\sigma_1(j)+g\sum_{j=1}^{n-1}\sigma_3(j)\sigma_3(j+1)+x[\sigma_3(1)+\sigma_3(n)]. \tag{3}$$

Let us denote the lowest eigenvalue of h_n by $-\lambda_n$ and use L/n copies of its corresponding eigenvector to build a candidate for the vacuum of Eq. (1). The correspondence $i\to j$ between the two sets of points is given by $i\equiv j \pmod n$. The resulting ground-state energy density E_n can be expressed as

$$-nE_n=\lambda_n-x\frac{\partial\lambda_n}{\partial x}+\frac{g}{4}\left(\frac{\partial\lambda_n}{\partial x}\right)^2 \tag{4}$$

for every $n\geq 2$. This follows from Eqs. (3) and (1) by substracting from λ_n the expectation value of $x[\sigma_3(1)+\sigma_3(n)]$ and adding the missing interaction term between adjacent boxes. At this point we vary the parameter x until a minimum is found,

$$\frac{\partial E_n}{\partial x}=0,\quad \frac{\partial^2 E_n}{\partial x^2}>0. \tag{5}$$

In the Appendix we prove that the solution of these conditions is

$$x_n=\frac{g}{2}\frac{\partial\lambda_n}{\partial x_n}. \tag{6}$$

Its physical meaning is that the best x of Eq. (3) is given by $g\langle\sigma_3\rangle$ of the nearest neighbor in the adjacent box. Substituting it back into Eq. (4) we find

$$-nE_n=\lambda_n-\frac{x_n^2}{g}. \tag{7}$$

The case $n=1$ is different because every point has two neighbors which belong to different boxes. Here

$$-h_1=\sigma_1+x\sigma_3, \tag{8}$$

and

$$-E_1=\lambda_1-x\frac{\partial\lambda_1}{\partial x}+g\left(\frac{\partial\lambda_1}{\partial x}\right)^2. \tag{9}$$

The variation procedure leads to

$$x_1=2g\frac{\partial\lambda_1}{\partial x}, \tag{10}$$

$$-E_1=\lambda_1-\frac{x_1^2}{4g}. \tag{11}$$

The case $n=1$ is just the mean-field approach in which one represents the vacuum by the product $\prod_{i=1}^{L}|i\rangle$. Starting with this proposition one searches for the same state for every i which will lead to a minimal E_1. This is analogous to the Hartree approach in atomic physics and leads to h_1 of Eq. (8) and E of Eq. (11). Our method is a generalization of this mean-field approach leading to the lowest energy of a ground-state wave function with periodicity n.

The case $n=1$ is, of course, the simplest as well as the worst approximation. $\lambda_1=(1+x^2)^{1/2}$ and Eq. (10) have a nontrivial solution $g=\frac{1}{2}(1+x^2)^{1/2}$ only for $g\geq\frac{1}{2}$. $g_c=\frac{1}{2}$ is the predicted critical point in this approximation. Below this point the minimal energy is given by $x=0$ and $E_1=-1$, i.e., σ_1 is diagonalized at every point. Above $g=\frac{1}{2}$ we find that σ_3 acquires a vacuum expectation value

$$\langle\sigma_3\rangle=\frac{x}{2g}=\pm\left(1-\frac{1}{4g^2}\right)^{1/2}.$$

$\langle\sigma_3\rangle$ is the order parameter of this problem, and we see that it has the characteristic $\frac{1}{2}$ power law of the mean-field approximation.

The case $n=2$ has $x=0$ and $-2E=(4+g^2)^{1/2}$ below $g_c=0.585$. Above this point a nontrivial solution is obtained with $x\neq 0$. The various cases $n=1,2,3$ are shown in Fig. 1 where we compare the values of E and $\langle\sigma_3\rangle$. The main qualitative changes are that g_c increases and E_n decreases with increasing n, thus exhibiting a monotonic improvement of the approximation. The phase transition is always continuous because it follows from Eqs. (5) and (7) that near $x=\epsilon\to 0$

$$\left.\frac{dE_n}{dg}\right|_{x=\epsilon}-\left.\frac{dE_n}{dg}\right|_{x=0}=-\frac{\epsilon^2}{ng^2}\to 0. \tag{12}$$

Although this method finds a continuous phase transition it is slow in providing a satisfactory detailed description of the physics near the critical point. For this purpose one should use it as a starting point of a renormalization-group calculation. The remarkable power of this variational method is manifested in the region $g>1$ where $\langle\sigma_3\rangle\neq 0$ in the exact solution. It is here where we observe a rapid convergence to the exact value of E. This is shown in Fig. 2. Note that whereas around $g\approx 0.6$ the curve of E_3 is quite far from E, they become very close above $g=1$. To have a clearer comparison over a wide range we plot the dual reflection of E_3, i.e., $gE_3(g^{-1})$, in the range $0<g<1$. This corresponds to the vacuum energy density of the model[2]

$$-H=\sum_i\tau_3(i)\tau_3(i+1)+g\sum_i\tau_1(i), \tag{13}$$

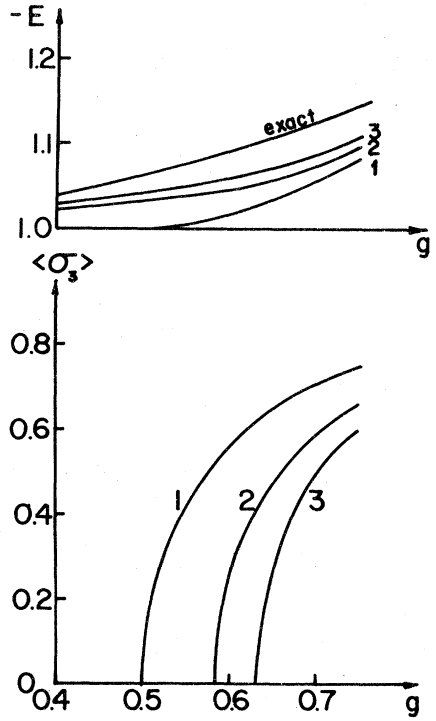

FIG. 1. Results for the order parameter and vacuum energy density for the $D=1$ Ising model. The variational method was used with boxes of sizes $n=1,2,3$.

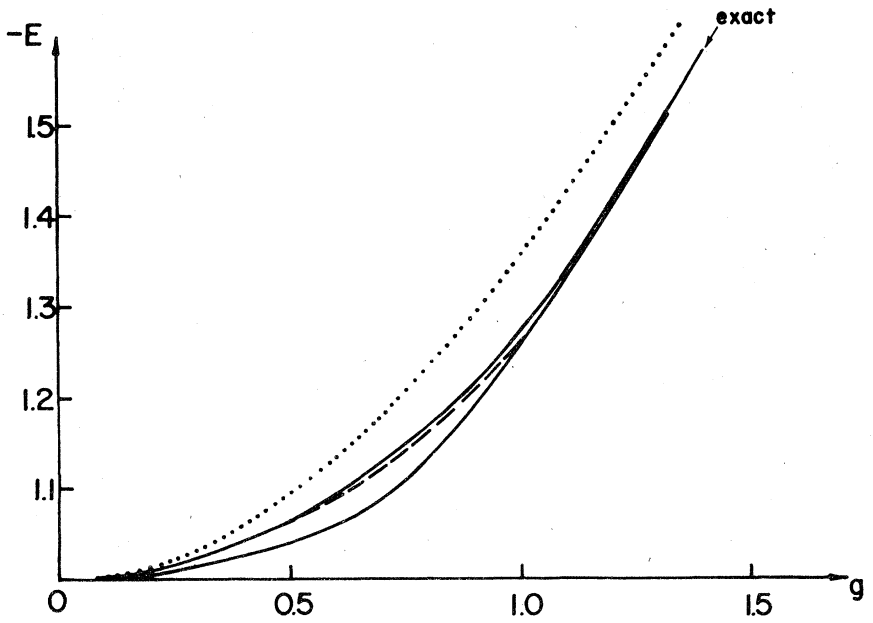

FIG. 2. Comparison of E_3, the vacuum energy density for box of size $n=3$ with the exact result of the $D=1$ Ising problem. The dashed curve is the dual reflection of E_3 which also serves as an upper limit to the true E. The dotted curve is a lower limit on E derivable from a box of size 3 using a (nonvariational) method described in Sec. IV.

where $\tau_{1,3}$ are Pauli matrices defined on the links of the lattice on which Eq. (1) was defined. The energy densities of the Hamiltonians (1) and (13) are equal by duality, but the variation approximation to Eq. (1) is useful where $\langle\sigma_3\rangle\neq 0$, i.e., $g>1$, whereas the same approximation applied to Eq. (13) works best when $\langle\tau_3\rangle\neq 0$, i.e., $g<1$. This way we obtain from E_3 an upper bound on $E(g)$ whose worst deviation from the exact result (at $g=1$) is less than 1%.

III. $Z(N)$ MODELS

A mean-field technique works usually better if the dimension is increased. The same is true for our variation method. Analyzing the Ising model of Eq. (1) for $D=2$, i.e., a two-dimensional square lattice, we find smaller energy differences between the successive approximations. The method we follow is quite the same but now the approximation is characterised not merely by the size of the cluster but also by its shape and the way one tiles the two-dimensional lattice with it. In Fig. 3 we present the results for the energy densities E_1, E_2, and E_4 of the Ising problem corresponding to the three cases of a single-site box, two sites, and a square of four sites. Since the three configurations fit successively into one another it is easy to prove that their corresponding ground-state energies have to obey $E_1\geq E_2\geq E_4$ over the whole range of g. The differences between these values are much bigger when g is very small indicating once again that the method is best in the region where the order parameter is large. In all cases the predicted g_c is not very far from the result $g_c\approx 0.33$ which is based on several perturbative calculations.[3]

Let us turn now to an application of our variation method to a $Z(N)$ theory. In $D=2$ space dimensions the local gauge-invariant $Z(N)$ theory is dual to a $Z(N)$ spin theory. Let us define the local gauge-invariant Hamiltonian[4]

$$-H=g\sum_l (P_l+P_l^\dagger) + \sum_p (Q_{p1}^\dagger Q_{p2}^\dagger Q_{p3} Q_{p4}+\text{H.c.}) \tag{14}$$

in terms of link operators P and Q which obey the $Z(N)$ algebra

$$P^\dagger P=Q^\dagger Q=1,\quad P^N=Q^N=1,\quad P^\dagger Q P=e^{2i\pi/N}Q\,. \tag{15}$$

The second term of Eq. (14) is the sum of products of Q_l over links which surround a plaquette. Each such product may be regarded as an operator of the dual lattice. Similarly, P_l may be defined in terms of operators S associated with plaquettes which intersect at that link:

$$Q_{p1}^\dagger Q_{p2}^\dagger Q_{p3} Q_{p4}=R_p,\quad P_l=S_{l+}^\dagger S_{l-}\,. \tag{16}$$

R and S obey the same algebra as P and Q and

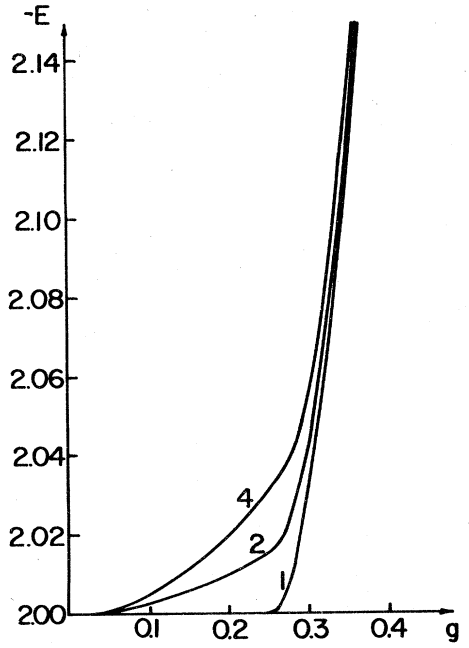

FIG. 3. Comparison of three different estimates of the vacuum energy density of the $D=2$ Ising problem. 1, 2, and 4 refer to basic clusters (boxes) of the corresponding number of sites. 4 represents a square box. The successive improvements of E show also an increase of g_c towards the correct value of 0.33.

the Hamiltonian dual to Eq. (14) may be written as

$$-H=g\sum_{\langle pq\rangle}(S_p^\dagger S_q+S_q^\dagger S_p)+\sum_p (R_p+R_p^\dagger), \tag{17}$$

which is a straightforward generalization of the Ising model Eq. (1) for $Z(N)$ spins.

Using a variational mean-field approach we are led to the single-site Hartree Hamiltonian

$$-h_1=x(S^\dagger+S)+iy(S^\dagger-S)+R^\dagger+R, \tag{18}$$

where (for $D=2$)

$$x=4g\,\mathrm{Re}\langle S\rangle,\quad y=4g\,\mathrm{Im}\langle S\rangle. \tag{19}$$

Equation (19), which may be anticipated from the variational approach, can be derived by analyzing the energy density of the trial state which is composed of the lowest eigenfunction of h in every box:

$$-E_1=\lambda-x\frac{\partial\lambda}{\partial x}-y\frac{\partial\lambda}{\partial y}+g\left(\frac{\partial\lambda}{\partial x}+i\frac{\partial\lambda}{\partial y}\right)\left(\frac{\partial\lambda}{\partial x}-i\frac{\partial\lambda}{\partial y}\right). \tag{20}$$

The conditions (see the Appendix)

$$x=2g\frac{\partial\lambda}{\partial x},\quad y=2g\frac{\partial\lambda}{\partial y}, \tag{21}$$

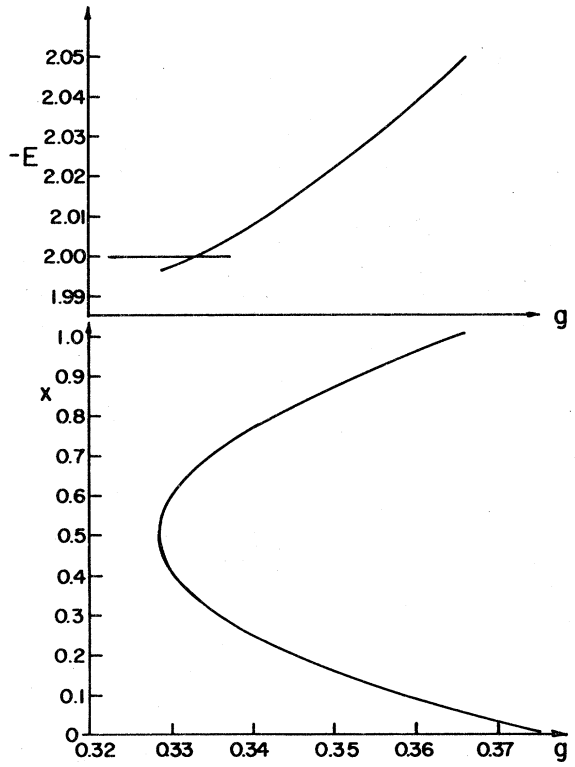

FIG. 4. The mean-field approximation for the $Z(3)$ problem which shows the character of a first-order phase transition. The results are shown for $D=2$ space dimensions. The exceptional structure of $x(g)$ which is responsible for the first-order character is discussed in the text. The two branches of E correspond to the trivial ($x=0$) and nontrivial $x(g)$ solutions.

which are the same as Eq. (19), guarantee a local minimum of E. Using Eq. (21) we can rewrite Eq. (20) as

$$-E_1=\lambda-\frac{x^2+y^2}{4g}. \tag{22}$$

Let us first fix $r^2=x^2+y^2$ and vary $\varphi=\arctan(y/x)$. The minimum is then determined only by λ. In fact there are N equivalent minima because the similarity transformation $R^\dagger hR$ transforms $\varphi\to\varphi+2\pi/N$. This shows the N-fold degeneracy of the vacuum. One such minimum lies at $\varphi=0$, i.e., $y=0$, as one may prove to all orders of perturbation theory in x^{-1}. We are therefore left with the task of finding the optimal x.

The case $N=2$ is the Ising model studied above. Its mean-field solution leads to the connection $x^2=16g^2-1$ starting at $g_c=0.25$. The $Z(4)$ theory has the same behavior. However for $N=3$ one encounters the surprise exhibited in Fig. 4: the relation $x=2g\partial\lambda/\partial x$ leads to a double-valued solution over a small range of g and the branch which

describes a minimum crosses the trivial solution ($x=0$ and $E_1=-2$) at a finite x value with a nonvanishing derivative. In other words, E_1 of $Z(3)$ exhibits a first-order phase transition. This is unique to $N=3$. For $N\geq 5$ we find that

$$\frac{dg}{dx}=0,\quad \frac{d^2g}{dx^2}>0,\quad \text{at } x=0 \tag{23}$$

as for $N=2$ and 4. This guarantees that the new minimum starts indeed at $x=0$ and Eq. (12) predicts then a continuous phase transition.

Since we are interested in the properties near $x=0$ we may employ perturbation arguments in x to derive Eq. (23), even though we discuss finite g values. Using fourth-order perturbation theory we find for $N\geq 5$

$$\lambda=2+\frac{x^2}{1-\cos\delta}-\frac{x^4(1+\cos\delta-2\cos2\delta)}{4(1-\cos2\delta)(1-\cos\delta)^3}, \tag{24}$$

where $\delta=2\pi/N$. Expanding g near $x=0$ we find then

$$g=\frac{x}{2d\lambda/dx}$$

$$\approx\frac{1-\cos\delta}{4}+\frac{x^2}{8}\frac{1+\cos\delta-2\cos2\delta}{(1-\cos\delta)(1-\cos2\delta)}, \tag{25}$$

which leads to

$$g_c=\frac{1-\cos\delta}{4}\underset{N\to\infty}{\sim}\frac{\pi^2}{2N^2}$$

and to Eq. (23). For $N<5$, λ acquires other terms. In particular, for $N=3$ there exists an x^3 term in λ which leads to the exceptional behavior of Fig. 4.

The mean-field results are consistent with what is known about the $D=2$ gauge theories. In particular, in the limit $N\to\infty$ Eq. (14) turns into the U(1) gauge theory in $2+1$ dimensions[4] with $g\delta^2$ playing the role of e^4. Equation (25) leads then to the expected result of a single phase in this limit. The correspondence between the gauge and spin models [Eqs. (14) and (17)] holds only at $D=2$. The above method can, however, be applied to the global $Z(N)$ theory, Eq. (17), in any space dimension D: h_1 remains unchanged but the x and y parameters have to be redefined as

$$x+iy=2Dg\langle S\rangle, \tag{26}$$

reflecting the effect of the neighbor sites. As a result the energy density becomes

$$-E_1=\lambda-\frac{x^2+y^2}{2Dg}. \tag{27}$$

Since λ is only a function of x and y, the mean-field solution remains the same up to a rescaling of the coupling g. Its implications are, however, unacceptable at $D=1$ where it is known that $Z(3)$ possesses a second-order phase transition (at $g_c=1$) and the $Z(N)$ model for $N\geq 5$ has three phases.[5] To see how such changes can reflect themselves in our approach we study the $Z(3)$ model at $D=1$ with boxes of size $n=2$ and 3. The box Hamiltonians are the generalizations of Eq. (3):

$$-h_n=\sum_{j=1}^{n}(R_j+R_j^\dagger)+g\sum_{j=1}^{n-1}(S_j^\dagger S_{j+1}+S_{j+1}^\dagger S_j)$$

$$+x(S_1+S_1^\dagger+S_n+S_n^\dagger), \tag{28}$$

where we limited ourselves already to the case $y=0$. Applying the variation procedure we find for the nontrivial solution,

$$-nE_n=\lambda_n-\frac{2x_n^{\,2}}{g}, \tag{29}$$

where

$$x_n=\frac{g}{4}\frac{\partial\lambda_n}{\partial x_n}. \tag{30}$$

The calculation of λ_n involves the diagonalization of a 4×4 matrix for $n=2$ and a 10×10 matrix for $n=3$. The results are displayed in Fig. 5. It is evident that g_c indeed increases towards $g=1$ and the jump in the derivative of the energy density $\Delta dE_n/dg$ decreases with n. Its values are 0.51, 0.17, and 0.12 for $n=1,2,3$, respectively. We again employ self-duality to obtain a better estimate of E in the region $g<1$. This serves as a reminder that the phase-transition point for each E_n is where the approximation is the worst.

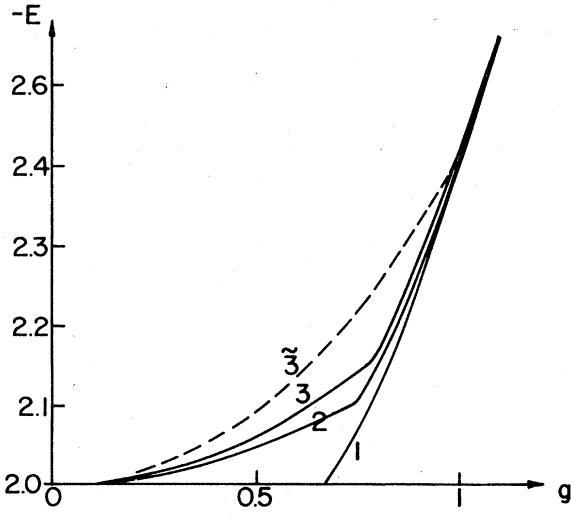

FIG. 5. Consecutive improvements on the $Z(3)$ vacuum energy density for $D=1$ show a decrease in the discontinuity of dE/dg. $\tilde{3}$ denotes the dual reflection of E_3.

Nonetheless, it is gratifying to see that $\Delta dE_n/dg$ decreases rapidly. It is interesting to note that in the $D=2$ problem, $\Delta dE_n/dg$ obtains the values 1.09 and 0.94 for $n=1$ and 2, respectively. Comparing with the rapid decrease found for $D=1$ this seems to imply that the mean-field result for $D=2$ shows the correct qualitative features. Monte Carlo calculations in $2+1$ dimensions have indeed shown a first-order transition for the $Z(3)$ model.[6]

IV. SUMMARY AND DISCUSSION

We have described a variation procedure whose main advantage is its rapid convergence in the ordered phase. This is because the order parameter played a key role in this procedure. If one wants to apply such a method to a local gauge theory one should first transform it into an equivalent model which allows one to rely on local operators which develop vacuum expectation values. In $D=2$ space dimensions we have used duality to transform the pure gauge theory into a spin theory to which the method can be applied. For $D=3$ this is no longer possible. One can, however, treat gauge theories with matter in this way. As an example let us describe the situation for the $Z(2)$ gauge and matter theory. Its Hamiltonian is given by[7]

$$-H=t\sum_l \sigma_1(l)+\frac{1}{t}\sum_p[\sigma_3\sigma_3\sigma_3\sigma_3](p)$$
$$+\frac{1}{x}\sum_i \tau_1(i)+x\sum_l[\tau_3\sigma_3\tau_3](l), \tag{31}$$

where $[\sigma_3\sigma_3\sigma_3\sigma_3](p)$ denotes the product of four σ_3 link operators around a plaquette and $[\tau_3\sigma_3\tau_3](l)$ is the product of a σ_3 link operator and the two vertex operators τ_3 associated with the end points of the link. τ_1 and τ_3 are Pauli matrices associated with all vertices and representing the matter field. The unitary gauge is given by

$$\tau_3=1,\quad \tau_1=\prod_{l\ni i}\sigma_1(l), \tag{32}$$

where $\prod_{l\ni i}$ represents a product over all links which intersect at the vertex i. This leads to the Hamiltonian

$$-H=t\sum_l \sigma_1(l)+\frac{1}{t}\sum_p[\sigma_3\sigma_3\sigma_3\sigma_3](p)$$
$$+\frac{1}{x}\sum_i\prod_{l\ni i}\sigma_1(l)+x\sum_l\sigma_3(l) \tag{33}$$

from which all gauge freedom was removed. Only in the limit $x\to 0$ it becomes again the pure $Z(2)$ gauge theory.

A mean-field approach to this problem was presented in Ref. 8. It was very successful in exhibiting the line of first-order transitions which exist in this model.[9] This is a border line between two regions where the operators $\sigma_{1,3}$ obtain different vacuum expectation values. From the models discussed in Secs. II and III one may indeed expect that the variation method should be successful in this case. The method does not work well at a critical point because it is based on a wave function which does not allow large-scale fluctuations, However, at a first-order transition point the large-scale fluctuations do not play a crucial role and the system makes a sudden transition from one kind of order to another kind. Hence the variation method should be more appropriate here than, for instance, a renormalization-group approach.

It is of interest to compare the variational approach with another method which provides a lower (rather than upper) bound on E. This consists of breaking the given H into box Hamiltonians in such a way that H becomes the direct sum of these Hamiltonians. Thus, for example, in the $D=1$ Ising problem, we can define

$$-\bar{H}_n=\frac{1}{n}\sum_{j=1}^{n}\sigma_1(j)+\frac{1}{n-1}g\sum_{j=1}^{n-1}\sigma_3(j)\sigma_3(j+1). \tag{34}$$

If the first site of this finite chain is mapped onto the site i of Eq. (1), then

$$H=\sum_i \bar{H}_n(i), \tag{35}$$

where we assume periodic boundary conditions before the length of the chain is taken to infinity. $\bar{E}_n$, the lowest eigenvalue of $\bar{H}_n$, is a lower bound on E,

$$E\geq\bar{E}_n. \tag{36}$$

The example of $\bar{E}_3$ is shown in Fig. 2. $\bar{E}_3$ and E_3 are comparable in qualtity where $x=0$, but once the $x\neq 0$ solution of E_3 takes over it becomes a much better estimate. Around $g=1$, E_3 is already an order of magnitude closer to E than $\bar{E}_3$. The induced interaction terms and the variation procedure are responsible for this incredible improvement in a finite-matrix approach to the infinite-lattice problem. In fact the variation procedure effectively introduces the infinity of the lattice into the finite box Hamiltonian. Clearly, no finite lattice problem can exhibit a real phase transition. Therefore, none of the $\bar{E}_n$ possess a phase-transition singularity, whereas the E_n solutions of the variation procedure acquire this singularity either at the origin of x (for a continous transition) or at a finite value of x for a

first-order transition.

Finally, we should comment about the symmetry of the problem and its spontaneous breaking. Clearly, Eq. (1) possesses the global symmetry

$$\sigma_1 \to \sigma_1, \quad \sigma_3 \to -\sigma_3 . \tag{37}$$

In the box Hamiltonians (3) this has to be augmented by

$$x \to -x . \tag{38}$$

This symmetry is finally manifested in the dependence of E_n on x^2 in the Ising problem. The $Z(N)$ problem has an analogous N-fold symmetry and its E_n has N equivalent minima in a circle of fixed $r^2 = x^2 + y^2$. In other words, the global symmetry of H reflects itself as an explicit symmetry in the dependence of E_n on the parameters which were introduced in h_n.

Svetitsky *et al.*[10] have used a box Hamiltonian with symmetry-breaking terms as a starting point for a renormalization-group calculation. They have restored the symmetry by keeping a symmetric set of wave functions in the iterative procedure of the renormalization group. Their work triggered our investigation. Our aim was, however, different—to propose a systematic approach which will be simple and transparent. The results prove that, indeed, using only a small cluster of points one can observe, understand, and estimate physical features of Hamiltonian lattice theories.

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APPENDIX

The purpose of this appendix is to supply proofs to some of the statements made in the text. Let us start with the Ising model whose box Hamiltonian was defined in Eq. (3) to be

$$-h_n = \sum_{j=1}^{n} \sigma_1(j) + g \sum_{j=1}^{n-1} \sigma_3(j)\sigma_3(j+1) + x[\sigma_3(1) + \sigma_3(n)] . \tag{A1}$$

This expression is invariant under the interchange (parity)

$$\sigma(j) \to \sigma(n-j) . \tag{A2}$$

Hence the eigenstates of h_n will have a definite parity. In both extreme ends of parameter space ($0 \leq g \leq \infty$), the ground state has positive parity. Since this property is not changed by perturbation theory, the ground state will always have positive parity. As a result

$$\langle \sigma_3(1) \rangle = \langle \sigma_3(n) \rangle , \tag{A3}$$

where the averaging is always done in the vacuum. Denoting by λ the highest eigenvalue of $-h_n$ and using

$$\frac{\partial \lambda}{\partial x} = \langle \sigma_3(1) + \sigma_3(n) \rangle , \tag{A4}$$

which follows from Eq. (A1) we obtain

$$\frac{1}{2} \frac{\partial \lambda}{\partial x} = \langle \sigma_3(1) \rangle = \langle \sigma_3(n) \rangle . \tag{A5}$$

This property was used in establishing the physical meaning of the parameter x.

Regarding x still as a free parameter we obtained in Eq. (4) the expression for the energy density

$$-nE_n = \lambda - x \frac{\partial \lambda}{\partial x} + \frac{g}{4} \left(\frac{\partial \lambda}{\partial x} \right)^2 . \tag{A6}$$

The conditions for a local minimum of E_n are

$$-n \frac{\partial E_n}{\partial x} = -x \frac{\partial^2 \lambda}{\partial x^2} + \frac{g}{2} \frac{\partial \lambda}{\partial x} \frac{\partial^2 \lambda}{\partial x^2} = 0 , \tag{A7}$$

$$-n \frac{\partial^2 E_n}{\partial x^2} = \frac{\partial^3 \lambda}{\partial x^3} \left(-x + \frac{g}{2} \frac{\partial \lambda}{\partial x} \right) + \frac{\partial^2 \lambda}{\partial x^2} \left(-1 + \frac{g}{2} \frac{\partial^2 \lambda}{\partial x^2} \right) < 0 . \tag{A8}$$

Since λ is the highest eigenvalue of the Hermitian matrix $-h_n$, it obeys

$$\frac{\partial^2 \lambda}{\partial x^2} \geq 0 . \tag{A9}$$

The equality is satisfied only in the extreme limit $g \to \infty$. Therefore, the solution of Eq. (A7) has to obey

$$x = \frac{g}{2} \frac{\partial \lambda}{\partial x} , \tag{A10}$$

which is Eq. (6) in the text. For condition (A8) to be satisfied too, one has to simultaneously have

$$\frac{g}{2} \frac{\partial^2 \lambda}{\partial x^2} < 1 . \tag{A11}$$

As $g \to \infty$ (where $x \to g$) one finds by perturbation

expansion in g^{-1} that $\frac{1}{2}g\partial^2\lambda/\partial x^2 \to 0$. Reducing g, the inequality (A11) continues to be obeyed down to a point where $\partial^2 E_n/\partial x^2 = 0$. This is usually the point where the trivial solution $x = 0$ takes over. If not, a first-order transition to the trivial solution occurs before that point is reached, as in the $Z(3)$ case shown in Fig. 4.

Inserting Eq. (A10) into (A6) we obtain

$$-n E_n = \lambda - \frac{x^2}{g}. \tag{A12}$$

The two functions of Eq. (A6) and Eq. (A12) are equal only at the solution (A10). Nonetheless, one can also use E_n of Eq. (A12) as the function to be minimized. Its first derivative leads directly to Eq. (A10) and its second derivative is positive if Eq. (A11) is satisfied. Hence the expression (A6) and (A12) [or Eqs. (4) and (7) of the text] are equivalent although they are different functions of x and g.

Similar arguments hold for more complicated cases. Thus in the mean-field calculation of $Z(N)$ we obtain from Eq. (20) the following necessary conditions for a minimum:

$$-\frac{\partial E_1}{\partial x} = \left(2g\frac{\partial\lambda}{\partial x} - x\right)\frac{\partial^2\lambda}{\partial x^2} + \left(2g\frac{\partial\lambda}{\partial y} - y\right)\frac{\partial^2\lambda}{\partial x\partial y} = 0,$$

$$-\frac{\partial E_1}{\partial y} = \left(2g\frac{\partial\lambda}{\partial x} - x\right)\frac{\partial^2\lambda}{\partial x\partial y} + \left(2g\frac{\partial\lambda}{\partial y} - y\right)\frac{\partial^2\lambda}{\partial y^2} = 0. \tag{A13}$$

Here λ is the highest eigenvalue of the Hermitian matrix $-h_1$ of Eq. (18) and, as such, obeys

$$\frac{\partial^2\lambda}{\partial x^2} \geq 0, \quad \frac{\partial^2\lambda}{\partial y^2} \geq 0, \quad \frac{\partial^2\lambda}{\partial x^2}\frac{\partial^2\lambda}{\partial y^2} - \left(\frac{\partial^2\lambda}{\partial x\partial y}\right)^2 \geq 0. \tag{A14}$$

These inequalities (equality holds only in the extreme limit of g) ensure that Eq. (A13) can be solved only by

$$2g\frac{\partial\lambda}{\partial x} = x, \quad 2g\frac{\partial\lambda}{\partial y} = y, \tag{A15}$$

which is the same as Eq. (21). The further conditions for a stable minimum are best checked by an explicit calculation which also shows if the local minimum wins over the trivial solution, $x = y = 0$, which is valid in a range of small g.

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